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Photonic crystals with tunable band gap based on infilled and inverted opal-silicon composites

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Abstract. Three-dimensional opal-Si composites with both direct (a variable extent of filling of opal voids with Si) and inverted structures have been synthesized. A structural analysis of these fabricated systems is performed. Reflectance spectra from the surface (111) of the composites are measured. Observed spectral features are interpreted as a manifestation of the direction [111] photonic band gap that is tunable in position and width in the visible and near-infrared spectral ranges.

Introduction

Photonic crystals are structures in which the dielectric constant is modulated with a period comparable to wavelength of light and a photonic band gap (PBG) occurs in the electromagnetic spectrum as a result of Bragg diffraction at the edge of Brillouin zone [1]. If there exist a complete PBG, light propagation is inhibited in any direction inside the crystal within the spectral range of the PBG. This effect is believed to be crucial for potential applications of photonic crystals in optical communication, laser physics and quantum computing.

Artificial opals are considered as promising materials with photonic-crystal properties. The opals have a structure with the fcc lattice formed by close-packed amorphous silica spheres with diameters 150 to 1000 nm. Voids between the spheres may occupy up to 26% of total volume. This allows to change the material parameter $\eta = \sqrt{\varepsilon_v/\varepsilon_s}$ by introducing various fillings into the voids. (Hereafter, ε_s and ε_v designate dielectric constants of bulk materials, respectively, inside and outside of the space that were occupied in bare opal by silica spheres, $\eta = \max\left(\sqrt{\varepsilon_v/\varepsilon_s}, \sqrt{\varepsilon_s/\varepsilon_v}\right)$ being referred to as optical contrast when ε_v and ε_s are real values [1]). According to a theoretical estimation the complete PBG may open up at $\eta \geq 2.8$ [2].

This work is aimed at synthesizing opal-Si composites with direct (infilled with Si) and inverted (SiO_2 spheres are removed from original opal-Si composite) opal structures and investigating their optical properties. This study is expected to conclude about the possibility of designing opal-Si composite based photonic crystals with a PBG whose position and width are tunable in a wide wavelength range, the tuning being provided by the variation of ε_v and ε_s. To verify these suggestions reflectance spectra from the synthesized composites were measured, and specific spectral features are found. Theoretically, the observed features were interpreted as a manifestation of the PBG for "one-dimensional" propagation of light waves in high-symmetry directions [111] of the periodic fcc dielectric structure.

1. Experimental

Opals with the sphere diameter of 230 nm are used as original matrices to synthesize opal-Si composites. Preliminary analysis by SEM shows that silica spheres are tangent (Fig. 1*a*).

Silicon was embedded in the opal voids by thermal decomposition of 5% SiH_4-Ar gas mixture [3]. This results in formation of uniformly thick silicon layer covering the surface of silica spheres (Fig. 1*b*). Developed technique allows us to change the fill factor of the opal voids by silicon gradually. The fill factor of the voids could be varied from 0 to 100% depending on deposition conditions. Thickness of a sample with 100% filling of voids reaches 0.4 mm. As-prepared samples are subjected to annealing at $T = 800^{\circ}$C and pressure 1 Torr in ambient atmosphere. SEM image of the inverted structure (the (111) surface) is shown in Fig. 1*c*. The inverted structure was obtained by etching out substance of an opal matrix (SiO_2) in an aqueous solution of HF. The samples selected for further investigations were about $5\times5\times0.4$ mm in size. For the inverted structures the ratio η is estimated to be approximately 3.5.

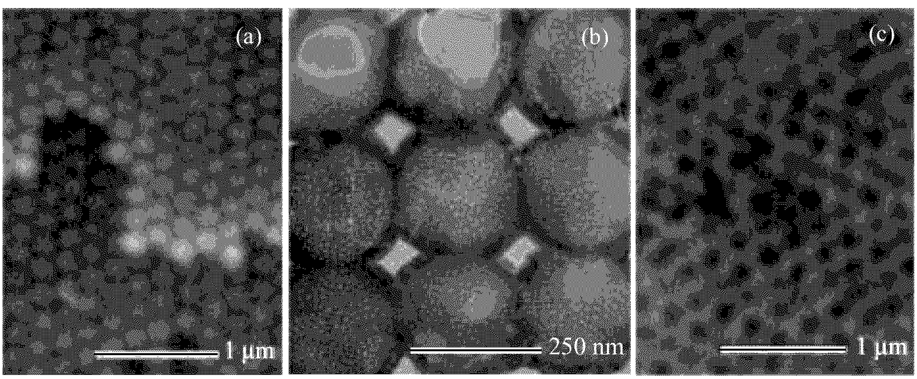

Fig. 1. SEM images of the (111) facet of bare opal (a), TEM image of the (100) plane of opal-Si composite (b), an inverted structure fabricated by selective etching out silica spheres from an opal-silicon composite (c).

2. Results and discussion

The problem of normal reflection of light from a photonic crystal may be considered as one-dimensional one based on the model of one-dimensional dielectric superlattice. Like in the light transmission problem [4], we describe the properties of opal-based structures using an "in-plane-averaged" dielectric constant

$$\varepsilon(z) = \varepsilon_s \cdot S(z) + \varepsilon_v \cdot [1 - S(z)].$$

Here, the coordinate z is measured along the normal vector to the (111) surface of a sample. Geometry of the structure is defined by the fcc lattice and the radius of spheres r. The function $S(z)$ is equal to the partial square belonging to the spheres in the cross-section with the coordinate z, therefore in our experiments $S(z)$ is periodic in the direction [111] with the period $d = r\sqrt{8/3}$. After calculating the function $S(z)$ for opal-based composites one-dimensional photonic bands as well as reflectance and transmittance spectra are calculated by transfer matrix technique within a model of periodically alternating ε-uniform layers [5].

Within the model [5] we have analyzed theoretically the effect of bulk refraction indices $\sqrt{\varepsilon_v}$ and $\sqrt{\varepsilon_s}$ on the reflectance spectra (Fig. 2*a*), the position and width of the stop bands (Fig. 2*b*). Used in these calculations are known complex values of silicon refraction index $\sqrt{\varepsilon_{Si}}$ taking into account optical dispersion and absorption. The refraction index $\sqrt{\varepsilon_s}$ of SiO_2 spheres was taken to be 1.37. Figure 2*b* presents theoretical estimations

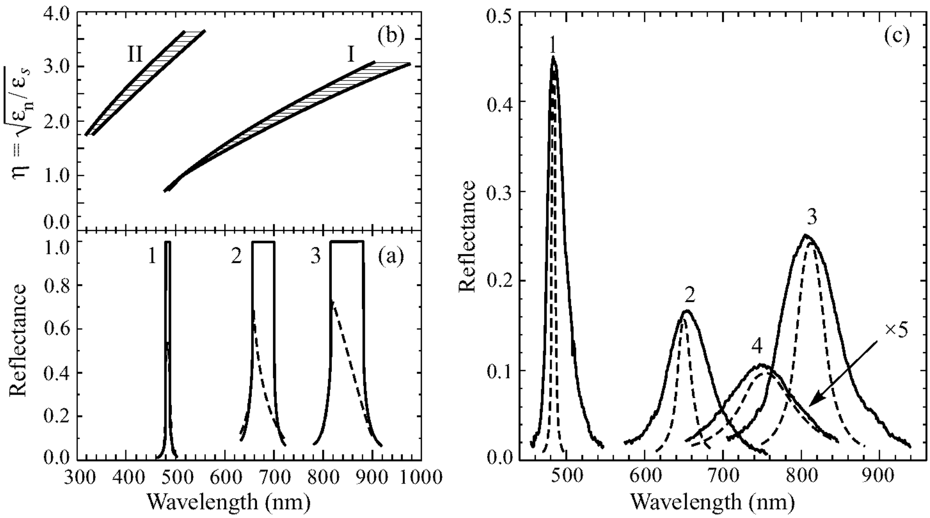

Fig. 2. Theoretical estimations of η−dependent (a) reflectance spectra from the (111) facet of opal-based composites at normal light incidence and (b) position and width of the two lower one-dimensional photonic band gaps (I and II). Solid curves are calculated in the absence of optical absorption, and dashed curves in making allowance for absorption. Curves 1 correspond to bare opal, 2 to opal partially filled with Si ($\sqrt{\varepsilon_{Si}}$=3.7), and 3 to opal completely filled with Si ($\sqrt{\varepsilon_{Si}}$=3.5). (c) Experimental (solid) and calculated (dashed) reflectance spectra at normal light incidence onto the (111) facet of various opaline composites specified in the text.

of one-dimensional stop bands. Widths and positions of the two lowest stop bands are shown as a function of η when optical absorption is neglected. Theoretical reflectance spectra corresponding to normal incidence of light onto the (111) surface (Fig. 2a) evidence existence of the stop bands (only data for the first stop band). Solid curves display total reflection resulted from existence of a stop band when optical absorption is neglected. In the presence of light absorption the shape of spectra changes, however, positions and widths of the spectral features stay approximately within the range of corresponding stop bands.

To verify the theoretical estimations we have measured the specular reflectance spectra from the (111) surface of synthesized composites. Additional light scattering resulted from the polydomain structure of opal samples was eliminated by applying optical microscope technique. Experimental reflectance spectra are shown by solid curves in Fig. 2c for the following samples: 1) bare opal, 2) opal partially filled with Si, 3) opal completely filled with Si, 4) silicon inverted opal. The spectra in Si-filled opals are found to shift to the long wavelength range and broaden as the parameter η increases. The observed peculiarities are confirmed by calculations (dashed curves in Fig. 2c) fitted to experimental data by small variation of the imaginary part of dielectric permittivity. This fitting procedure may be interpreted as introducing an extinction effect attributed to light scattering in the directions other than [111] inside the photonic crystal.

3. Conclusions

We have synthesized opal-Si composites with direct and inverse structure and studied, both experimentally and theoretically, their reflection spectra in a wide spectral range. Comparison of the experimental results with a theory, that predicts occurence of one-dimensional stop bands, has evidenced unambiguously that maxima in the observed reflection spectra are

due to Bragg diffraction of Bloch-type electromagnetic waves caused by one-dimensional periodic dielectric structure of investigated samples. Since the designed CVD technique enables us to control the fill factor of opal voids precisely it opens up an opportunity to create tunable Si-based photonic crystals with the prescribed position and width of the PBG.

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References

[1] *Photonic Band Gap Materials*, ed. by C. M. Soukoulis. Advanced Studies Institute of NATO, Ser. E, vol. 315 (Kluwer, Dordrecht, 1996).

[2] K. Bush and S. John, *Phys. Rev. E* **58**, 3896 (1998); A. Blanco, E. Chomski, S. Grabtcak, M. Ibisate, S. John, S. W. Leonard, C. Lopez, F. Mesequer, H. Miguez, J. P. Mondia, G. A. Ozin, O. Toader and H. M. van Driel, *Nature* **405**, 437 (2000).

[3] V. N. Bogomolov, V. G. Golubev, N. F. Kartenko, D. A. Kurdyukov, A. B. Pevtsov, A. V. Prokofiev, V. V. Ratnikov, N. A. Feoktistov, and N. V. Sharenkova, *Tech. Phys. Lett.* **24**, 326 (1998).

[4] Yu. A. Vlasov, V. N. Astratov, O. Z. Karimov, A. A. Kaplyanskii, V.N.Bogomolov and A.V.Prokofiev, *Phys. Rev. B* **55**, R13357 (1997); Yu. A. Vlasov, M. A. Kalitievskii and V. V. Nikolaev, *Phys. Rev. B* **60**, 1555 (1999).

[5] V. G. Golubev, V. A. Kosobukin, D. A. Kurdyukov, A. V. Medvedev and A. B. Pevtsov, *Semiconductors* **35**, (2001) (in press).